Importance of ORELA for Developing Nuclear Reaction Models

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Importance of ORELA for Developing Nuclear Reaction Models

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Abstract. Because of its excellent energy resolution, ORELA is particularly well suited for measurements in the resolved resonance region that impact nuclear reaction model calculations. These measurements allow the determination of average level widths, level densities, and cross sections for potential scattering and radiative capture. These quantities can be used to determine parameters in reaction models (such as the optical model and Hauser-Feshbach calculations) and to understand the limitations imposed on these models. Particular attention is given to the importance of improved experimental data to characterize intermediate structure (or doorway states).

INTRODUCTION

Continuous-energy ("white") neutron sources have been used since the 1950’s to measure the resonant structure in the energy dependence of neutron cross sections across the periodic table. In many applications the properties of these resonances (position, partial widths, total width) are used directly. In others, energy averages over the resonant structure are the important quantities; these energy averages determine the low-energy behavior of the nuclear optical model, which is a key ingredient in nearly all descriptions of nuclear reactions, including statistical models (e.g. Hauser-Feshbach) and distorted-wave Born approximation (DWBA) direct-interaction models. The measured average spacing of the s-wave resonances provides a critical check on the level densities used in statistical reaction models.

Since properties of individual resonances can be measured only over a limited energy range, two questions arise that affect the reliability and interpretation of the energy-averaged quantities derived from them: Have the resonances been adequately measured, with proper attention to missing resonances, separation of s- and p-wave resonances, and separation of total spins (if the target has nonzero spin)? If so, what is the energy interval over which the energy-averaged resonance parameters applies? The first question is experimental, and recent work at ORELA (e.g. [1] for \(^{35,37}\text{Cl}+n\)) has shown that significant improvement on older data can be made. The second question, which is theoretical, addresses the issue of intermediate structure, which can invalidate the conventionally-used forms of reaction models, such as the optical model and radiative capture. The importance of intermediate structure (frequently interpreted using the concept of doorway states [2]) can only be answered if the experimental data base is sound, and this is where ORELA can make significant contributions.

FROM RESONANCES TO THE OPTICAL MODEL

The s-wave strength function is defined as \(S_0 = \langle \Gamma \rangle / D\), where \(\langle \Gamma \rangle\) is the energy average of the reduced neutron widths of the observed s-wave resonances, and \(D\) is the corresponding average level spacing. This strength function can be connected to the optical model if the averaging interval is large enough to contain sufficient number of resonances, but small enough that the statistical distribution of these parameters may be considered uniform within the interval. The measured values of \(S_0\) are shown in Fig. 1, together with calculations from a recent spherical global optical potential [3], shown only in mass regions where a spherical model applies.

The peaks in the plot of \(S_0\) are well understood to correspond to the presence of single-particle s-wave shell model states appearing close to the neutron separation energies at particular mass values (for example, \(3 \, s_{1/2}\) near \(A \approx 60\)). What we want to emphasize here are the deviations from the optical-model predictions, either as scatter that exceeds the experimental error bars, or as a significant average deviation (as happens most prominently in the \(A \approx 110-130\) region).
If the experimental data are reliable, such deviations provide strong evidence that a treatment beyond the standard optical model is needed. In fact, the low values of $S_0$ near mass 120 have been interpreted [4] via the doorway-state model discussed in the next section.

Other useful quantities that can be determined from the resonance parameters also show similar gross structure as well as fluctuations from this average structure. These are the p-wave strength function $S_1$, and the potential scattering radius $R'$, which characterizes the smooth s-wave background between resonances. These are discussed and tabulated in the compilation of Mughabghab et al. [5, 6].

**FIGURE 1.** Experimental values of the s-wave strength function [7], compared with calculations using a global optical potential (Koning-Delaroche [3]) for spherical nuclei.

**INTERMEDIATE STRUCTURE AND DOORWAY STATES**

Intermediate structure refers to structure on an energy scale between that of the individual resonances seen in a high-resolution experiment and the separation between single-particle (shape) resonances such as those responsible for the gross structure seen in the s-wave strength function. An example of such structure is visible in the total neutron cross section of $^{56}$Fe (see Fig. 2), which shows evidence for structure with widths on the order of 100-200 keV.

The fluctuations in the strength functions (e.g. Fig. 1) and the intermediate structure seen in Fig. 2 are plausibly explained by the doorway-state hypothesis, in which the initial interaction of the neutron with the target is assumed to generate only two-particle, one-hole (2p1h) configurations of the compound system. These, in turn, damp into more complicated configurations, and still further interactions eventually reach the equilibrated compound nucleus. The theory of doorway states was developed in the 1960’s (see, for example, articles by Feshbach, Kerman, and Lemmer [2]) and Lane [8, 9]. If the doorways are well separated the strength functions (e.g. $S_0$) can be written as a sum over doorway resonances

$$
\frac{\Gamma}{D} \approx \frac{1}{2\pi} \sum_d \frac{\Gamma_d^\uparrow \Gamma_d^\downarrow}{(E - E_d)^2 + \frac{1}{4}\Gamma_d^2}.
$$

While the reduced neutron escape width $\Gamma_d^\uparrow$ is fairly easy to estimate, the damping width of the 2p1h states into more complicated states, $\Gamma_d^\downarrow$, is poorly known. If the doorways are very dense and highly overlapping, the standard energy-averaged reaction picture (including, for example, the optical model) applies. On the other hand, if the resonances are sparse and narrow enough to retain their identity, a more complicated treatment that treats the doorways explicitly is required.

There are thus challenges to both theory and experiment: For theory, calculations need to be carried out that adequately calculate both the spectroscopic configurations of the doorways and their damping widths. For experiment, the relevant data must be measured (and old measurements revisited) to ensure that the deviations such as those indicated above from simple models are in fact real.
RADIATIVE CAPTURE

We discuss here two types of data on radiative capture, 1) the total capture cross section averaged over many resonances; and 2) direct capture and related topics.

Total capture cross sections are important for applications to astrophysics, reactor physics, and stockpile stewardship. In many cases they are difficult or impossible to measure directly because the targets are unstable or hard to obtain; in this case modeling calculations (Hauser-Feshbach) must be used, and their parameters must be tuned to reproduce measurements on nearby stable nuclei. As an example, the author has carried out Hauser-Feshbach calculations in the actinides that agree to about 10% with measurements on nonfissile targets; applying similar techniques to the deformed rare earth nuclei yields discrepancies at the level of 30–50%, which is unsatisfactory. Improved measurements are clearly needed to separate experimental and modeling uncertainties, and ORELA has made significant progress in the last few years through rebuilding the setup for capture measurements.

Direct radiative capture, which appears as a background amplitude between resonances, needs to be understood for a number of applications to astrophysics and for data evaluation. Even though the size of the direct-capture background is so low that it is usually obscured by background effects in \((n, \gamma)\) measurements, its integral over an energy interval containing many resonances may be large enough to constitute a significant fraction of the total average cross section. However, the theoretical techniques for estimating the direct-capture background are not fully agreed upon: the original work of Lane and Lynn [11, 12] used a complex optical potential in an \(R\)-matrix context to describe the continuum state, while Cugnon and Mahaux [13] have argued that it is satisfactory to use a real potential. Recent calculations [14, 15] undertaken to clarify the role of direct capture in ORELA measurements on s-d shell nuclei have used a real potential, but have found significant effects from using an improved form of the electromagnetic operator plus a small contribution from semidirect capture (excitation of the giant dipole resonance). Results of these last calculations for thermal energy are shown in the first line of Table 1; they are in disagreement with other calculations by amounts up to a factor of about 2. Note that the experimental values (last line) will exceed the direct-capture value if there is a resonance near thermal energy, as is the case for \(^{35}\)Cl. To test the various formulations of direct capture theory, it would be desirable to devise an experiment at ORELA with sufficiently low backgrounds to identify the direct capture component unambiguously. Alternatively, subtracting the resonant contribution to the average capture, which can be measured at ORELA, from the total capture (resonant plus direct) measured by an activation technique could yield the direct component if sufficient control on the systematic errors can be gotten.

Direct neutron capture proceeds only to final nuclear states that have a wave-function component that looks like the target plus a neutron. The same spectroscopy applies to a \((d, p)\) stripping reaction, and consequently the direct capture cross section is proportional to the spectroscopic factor measured in a \((d, p)\) reaction. This rule applies to the capture cross sections in the s-d shell in Table 1. However, in some cases this rule is completely violated, as shown in Fig. 3 for \(^{57}\)Fe, in which the radiative capture and the \((d, p)\) spectroscopic factors show no correlation (or even an
TABLE 1. Direct-capture estimates of thermal neutron capture cross sections (in mb) for selected s-d shell nuclei, together with experimental values.

<table>
<thead>
<tr>
<th></th>
<th>19F</th>
<th>27Al</th>
<th>28Si</th>
<th>29Si</th>
<th>30Si</th>
<th>35Cl</th>
<th>37Cl</th>
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<tr>
<td>Raman-Lynn ‡</td>
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<td>116</td>
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<td>70</td>
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<tr>
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<td>169</td>
<td>119</td>
<td>107</td>
<td>43600</td>
<td>433</td>
</tr>
</tbody>
</table>

* Calculations from Ref. [14, 15]
† Calculations reported in Refs. [19, 1, 20]
‡ Experimental values from Refs. [21, 22], theory in Ref. [23].
§ Experimental values from Ref. [5] (27Al, 37Cl), [21] (19F), and [22] (28,29Si).

Uncertainties ≤ 3%.

anticorrelation). This behavior has been interpreted using a doorway-state model; in this picture it is no accident that the total cross section of Fe shows intermediate structure (Fig. 2). These results underline the importance of carefully identifying the regions of the periodic table where intermediate structure or doorway states may invalidate simple models for scattering or capture.

A related phenomenon, valence capture, predicts that there is a component of the radiative width in neutron resonances that is also proportional to the \((d, p)\) spectroscopic factor for the final state reached by gamma decay. This arises from mixing of the single-particle resonances (such as are seen in the strength functions) into the resonances. A review of this subject approximately 25 years ago [16] showed a mixed picture for the success of this model. One means of identifying the valence mechanism requires careful investigation of the correlation between neutron and gamma widths of observed resonances. Recent work at ORELA [17] on such correlations in resonances in \(^{88}\text{Sr}(n, \gamma)\) has shown that earlier experiments may have led to incorrect conclusions.

FIGURE 3. Comparison of \((n, \gamma)\) and \((d, p)\) strengths for final states in \(^{57}\text{Fe}\) [18].
CONCLUSIONS AND ACKNOWLEDGMENTS

Accurate measurements of resonance parameters carried out with the high precision of which ORELA is capable can play a key role in elucidating the role of intermediate structure. There is significant evidence, some of which has been shown here, that doorway states need to be taken seriously. Lack of understanding of their properties is potentially a fundamental limitation on the validity of the optical model at low energies, and consequently a fundamental limitation on our ability to extrapolate reaction-model calculations off the valley of stability.

Scatter in the currently available measurements of radiative capture cross sections in the unresolved resonance region suggests the presence of systematic errors that can be corrected by making measurements with the improved capture apparatus now available at ORELA.

This brief overview has focused on total cross section and capture measurements; other types of measurements that can be made at ORELA that may significantly improve reaction models include fission.

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REFERENCES